

TABLE 1. Continuous Self-Consistent Basicity Scale of Neutral Bases in Acetonitrile

Base	$pK_a(\text{AN})^b$	Directly measured ΔpK_a^a
1 4-MeO-C ₆ H ₄ P ₃ (dma)	31.99	
2 PhP ₃ (dma)	31.48	0.80
3 2-Cl-C ₆ H ₄ P ₃ (pyrr) ₃ NEt ₂	31.19	0.98
4 4-CF ₃ -C ₆ H ₄ P ₃ (pyrr)	30.50	0.70
5 2-Cl-C ₆ H ₄ P ₃ (dma) ₃ NEt ₂	30.16	0.32
6 2,5-Cl ₂ -C ₆ H ₃ P ₃ (pyrr) ₃ NEt ₂	29.16	1.01
7 4-CF ₃ -C ₆ H ₄ P ₃ (dma)	29.10	0.08
8 EtP ₁ (pyrr)	28.88	0.93
9 t-BuP ₁ (pyrr)	28.42	0.86
10 4-MeO-C ₆ H ₄ P ₂ (pyrr)	28.23	0.86
11 PhP ₂ (pyrr)	27.55	0.64
12 MeP ₁ (dma)	27.52	0.69
13 HP ₁ (pyrr)	27.01	0.60
14 t-BuP ₁ (dma)	26.98	1.59
15 PhP ₂ (dma)	26.46	0.55
16 TBD	26.03	0.46
17 HP ₁ (dma)	25.85	1.03
18 MTBD	25.49	0.99
19 2-Cl-C ₆ H ₄ P ₂ (pyrr)	25.42	0.08
20 DBU	24.34	1.05
21 4-NMe ₂ -C ₆ H ₄ P ₁ (pyrr)	23.88	0.45
22 4-MeO-C ₆ H ₄ P ₁ (pyrr)	23.12	0.77
23 PhP ₁ (pyrr)	22.34	0.74
24 PhP ₁ (dma)	21.25	1.09
25 4-Br-C ₆ H ₄ P ₁ (pyrr)	21.19	1.77
26 PhP ₁ (dma) ₂ Me	21.03	0.10
27 PhTMG	20.84	0.44
28 1-NaphthP ₁ (pyrr)	20.61	0.44
29 2-Cl-C ₆ H ₄ P ₁ (pyrr)	20.17	0.46
30 4-CF ₃ -C ₆ H ₄ P ₁ (pyrr)	20.16	0.46
31 2-Tol-1-BG	19.66	0.59
32 pyrrolidine	19.56	0.59
33 2-Cl-C ₆ H ₄ P ₁ (dma)	19.07	0.26
34 Et ₃ N	18.82	1.07
35 Proton Sponge	18.62	0.23
36 2,6-Cl ₂ -C ₆ H ₃ P ₁ (pyrr)	18.56	0.06
37 2,5-Cl ₂ -C ₆ H ₃ P ₁ (pyrr)	18.52	0.04
38 4-NO ₂ -C ₆ H ₄ P ₁ (pyrr)	18.51	0.02
39 4-Pyrr-Pyridine	18.33	0.17
40 4-NMe ₂ -Pyridine	17.95	0.65
41 2-NO ₂ -4-Cl-C ₆ H ₃ P ₁ (pyrr)	17.68	0.25
42 4-NH ₂ -Pyridine	17.62	0.08
43 2-NO ₂ -5-Cl-C ₆ H ₃ P ₁ (pyrr)	17.27	0.76
44 PhCH ₂ NH ₂	16.91	0.40
45 2-NO ₂ -4-CF ₃ -C ₆ H ₃ P ₁ (pyrr)	16.54	1.01
46 2-NH ₂ -Acridine	16.39	0.85
47 2-NH ₂ -1-Me-Benzimidazole	16.31	0.09
48 2-NH ₂ -Benzimidazole	16.08	0.84
49 2,3-(NH ₂) ₂ -Pyridine	15.24	0.27
50 2,4,6-Me ₃ -Pyridine	14.98	0.36
51 2,4-(NO ₂) ₂ -C ₆ H ₃ P ₁ (pyrr)	14.88	0.10
52 2,6-(NH ₂) ₂ -Pyridine	14.77	0.51

Table 1. (Continued)

Base	$pK_a(AN)^b$	Directly measured ΔpK_a^a									
53 2-NH ₂ -Pyridine	14.47	0.75									
54 2,6-Cl ₂ -4-NO ₂ -C ₆ H ₂ P ₁ (pyrr)	14.43		0.73						0.35		
55 4-MeO-Pyridine	14.23		1.55						0.22		
56 3-NH ₂ -Pyridine	14.17			0.34							
57 2,6-Me ₂ -Pyridine	14.13								0.05		
58 2,6-(NO ₂) ₂ -C ₆ H ₃ P ₁ (pyrr)	14.12	1.72									
59 2-Me-Pyridine	13.32										
60 Pyridine	12.53		0.77								
61 OEP	12.37	0.66									
62 4-MeO-Aniline	11.86		0.83	1.01							
63 2-methylquinolin-8-amine	11.54		0.31								
64 N,N-Me ₂ -Aniline	11.43		0.07								
65 Aniline	10.62		0.95								
66 2-Me-Aniline	10.50		0.77	1.15							
67 TPP	10.41	0.22									
68 5-NO ₂ -Benzimidazole	10.39			1.58							
69 TMP	10.15	0.43	0.85								
70 MePh ₂ P	9.96		0.47								
71 TCPP	9.94	0.03		1.07					0.90	0.23	
72 2-MeO-Pyridine	9.93								0.85		
73 1-Napht-NH ₂	9.77	0.16							0.60		
74 3-Cl-Pyridine	9.55	0.24		0.38						0.32	
75 4-Br-Aniline	9.43		0.11	1.37	0.12						
76 2,4-F ₂ -Aniline	8.39			1.06							
77 4-CF ₃ -Aniline	8.03	1.57		0.35							
78 2-Cl-Aniline	7.86		0.71	0.35		1.77			0.35		
79 3-NO ₂ -Aniline	7.68	0.20									
80 4-F-3-NO ₂ -Aniline	7.67	0.01							0.17		
81 2,6-(MeO) ₂ -Pyridine	7.64	0.05		0.04						0.07	
82 PhP ₃	7.61	0.04	0.88		1.51				0.07		
83 2-Cl-Pyridine	6.79	1.40		1.43					1.40		
84 4-NO ₂ -Aniline	6.22		0.57								
85 2,5-Cl ₂ -Aniline	6.21	0.01									
86 Ph ₂ NH	5.97	0.25	1.16			1.40					
87 2,6-Cl ₂ -Aniline	5.06	0.91									
88 2-NO ₂ -Aniline	4.80	1.30		1.18							
89 4-Cl-2-NO ₂ -Aniline	3.80		0.25								
			0.97								

^a The numbers on the arrows are the experimental ΔpK_a values from this work and our previous works.⁶⁻⁸ ^b Absolute pK_a values (see the Results).